CLAIMS

What is claimed is:

1. A secondary compound library produced by a method of screening a compound library or portion thereof by absorption, said method comprising:

(i) screening a primary compound library or portion thereof having a plurality of test samples containing isolated compounds or isolated mixtures of compounds per test sample by generating an *in vivo* absorption profile for each of said test samples from initial dose data and from *in vitro* bioavailability data comprising permeability and solubility data [, and optionally dissolution rate and transport mechanism data] for each of said test samples, wherein said absorption profile includes at least one of rate of absorption, extent of absorption, and concentration of a test sample; and

(ii) producing a secondary compound library comprising at least one compound from the primary compound library having a desired absorption profile.

2. The secondary compound library of claim 1, wherein said permeability data is obtained from a cell-based assay.

3. The secondary compound library of claim 1, wherein said solubility and said dissolution rate data is obtained from a chemical-based assay.

4. The secondary compound library of claim 1, wherein the absorption profile is generated for a mammalian system of interest, the system of interest is selected from the group consisting of the gastrointestinal tract, the eye, the nose, the lung, the skin, and the brain.

5. The secondary compound library of claim 1, wherein said primary compound library is selected from the group consisting of at least one of a natural library, a synthetic library, and a combinatorial library.

6. The secondary compound library of claim 1, wherein said *in vivo* absorption profile is generated by providing said initial dose data and said *in vitro* bioavailability data to a computer-implemented pharmacokinetic tool (PK tool), wherein said PK tool comprises an input/output system and a physiological model of a mammalian system of interest, wherein said input/output system and model carry out the steps of:

(i) receiving through the input/output system as input data, said initial dose data and said *in vitro* bioavailability data for one of said test samples; and

(ii) generating as output data a simulated *in vivo* absorption profile for said test sample.

7. The secondary compound library of claim 6, wherein said physiological model is for a mammalian system selected from the group consisting of gastrointestinal tract, eye, nose, lung, skin, and blood brain barrier.

8. The secondary compound library of claim 1, which further comprises: (iv) screening said secondary compound library by one or more properties in addition to absorption; (v) selecting compounds by one or more of said properties, and (vi) producing secondary compound libraries characterized by absorption, and one or more of said properties.

9. The method of claim 8, wherein said one or more properties in addition to absorption is selected from the group consisting of metabolism, toxicity and activity.

10. A method of screening a compound library or portion thereof by absorption, said method comprising:

(i) screening a compound library or portion thereof having a plurality of test samples containing isolated compounds or isolated mixtures of compounds per test sample by generating a predicted *in vivo* absorption profile for each of said test samples from initial dose data and from *in vitro* bioavailability data comprising permeability and solubility data for each of said test samples, wherein said predicted absorption profile is characterized by one or more of rate of absorption, extent of absorption, and concentration of a test sample for one or more physiological barriers to absorption of a mammalian system of interest, wherein said predicted *in vivo* absorption profile is generated by:

a. providing said initial dose data and said *in vitro* bioavailability data to a computer-implemented pharmacokinetic tool (PK tool) which comprises an input/output system and a physiological model of said

mammalian system of interest, wherein said input/output system and model work together to carry out the steps of:

b. receiving through the input/output system as input data, said initial dose data and said *in vitro* bioavailability data for one or said test samples; and

c. generating as output data a predicted *in vivo* absorption profile for said test sample; and

(ii) producing a secondary compound library comprising compounds having a desired absorption profile, whereby said compound library or portion thereof is screened by absorption.

11. The method of claim 10, wherein said physiological model is a mathematical model of said mammalian system comprising as operably linked components: (i) differential equations for calculating solubility and absorption of a test sample for one or more physiological segments of the mammal system of interest; and (ii) initial parameter values for the differential equations corresponding to physiological parameters and one or more selectively optimized adjustment parameters for one or more physiological segments of said mammal system of interest.

12. The method of claim 11, wherein said permeability data is derived from a cell-based assay.

13. The method of claim 12, wherein said solubility and said dissolution rate data is derived from a chemical-based assay.

14. The method of claim 11, wherein said mammalian system of interest is selected from the group consisting of the gastrointestinal tract, the eye, the nose, the lung, the skin, and the brain.

15. The method of claim 11, wherein said compound library is selected from the group consisting of a natural library, a synthetic library, and a combinatorial library.

16. The method of claim 11, wherein said physiological model is for a mammalian system selected from the group consisting of gastrointestinal tract, eye, nose, lung, skin, and blood brain barrier.

17. A secondary compound library produced by the method of claim 11.

18. The method of claim 11, which further comprises: (iv) screening said secondary compound library by one or more properties in addition to absorption; (v) selecting compounds by one or more of said properties, and (vi) producing one or more compound libraries characterized by absorption, and one or more of said properties.

19. The method of claim 18, wherein said one or more properties in addition to absorption is selected from the group consisting of metabolism, toxicity and activity.

20. A secondary compound library produced by the method of claim 19.